

COMPUTATIONS OF OPTIMAL TRANSPORT DISTANCE WITH FISHER INFORMATION REGULARIZATION

WUCHEN LI, PENGHANG YIN, AND STANLEY OSHER

ABSTRACT. We propose a fast algorithm to approximate the optimal transport distance. The main idea is to add a Fisher information regularization into the dynamical setting of the problem, originated by Benamou and Brenier. The regularized problem is shown to be smooth and strictly convex, thus many classical fast algorithms are available. In this paper, we adopt Newton's method, which converges to the minimizer with a quadratic rate. Several numerical examples are provided.

1. INTRODUCTION

Optimal transport distances among histograms play crucial roles in applications, such as image processing, machine learning, and computer vision [22, 27]. For example, the metric has been widely used in image retrieval problems [25]. The successful usage of the metric is mainly due to its many desirable theoretical properties, see [12, 27, 30]. However, the current computation speed is still not a satisfactory. On one hand, the problem usually relies on solving a very large dimensional linear program, whose dimension is quadratic in the support of the histograms. Such a large dimension makes the numerics cumbersome [10]. On the other hand, an optimal control formulation of the problem has been proposed, known as the Benamou-Brenier formula [1]. In this setting, the discretized problem is a constrained minimization, whose dimension is smaller than the one in a linear program. But its objective function is nonlinear, non smooth, and lacks strict convexity. It also has inequality constraints, i.e. the density functions are required to be non-negative. All above facts slow down the speed of computation [24].

Parallel to optimal transport, Schrödinger considered a similar problem in 1931 [17] (It is different from his famous Schrödinger equation). Nowadays, such a problem is understood in the context of optimal transport, which adds the Fisher information into the Benamou-Brenier formula [2, 5]. The Fisher information is a famous functional in statistical physics [13] and has interesting connections with diffusion processes and optimal transport distance [23, 30]. From the viewpoint of computation, it is the regularization term. The regularized problem enjoys many nice properties, e.g. its minimizer stays positive and converges to the one of original problem. We give a short review in section 2. However, it is not straightforward to apply this regularization into computations. The main obstacle here is that the spatial grids are no longer a length space (a space where one can define the lengths of curves). Thus many techniques in optimal transport can not be applied.

Key words and phrases. Optimal transport; Fisher information; Schrödinger bridge problem; Newton's method.

This work is partially supported by ONR grants N000141410683, N000141210838 and DOE grant de-sc00183838.

In this paper, we overcome the aforementioned difficulties using work in [7, 18], named discrete optimal transport (Similar work has been discussed in [6, 21]). Based on this, we form the Fisher information on spatial grids and apply it into the discretized Benamou-Brenier formula. The regularized minimization is proved to be smooth and strictly convex, which allows us to apply Newton's method [16]. Our approach has the following highlights: (1) It handles the inequality constraints by adding a "particular" barrier, which forces the minimizer in the interior (density function stays positive) and keeps the objective function smooth; (2) The regularized objective function is strictly convex and its Hessian matrix is sparse. These two facts make each update in the algorithm simple, with an overall quadratic convergence rate.

It is worth mentioning that, although the Fisher information is crucial in many disciplines [4, 13], its importance in computation is not well known yet. The Fisher information in variational problems was started by Edward Nelson [2, 23]. Our discretized problems share many similarities with Nelson's work. In addition, the regularizations in optimal transport have been discussed in the literature [4, 10, 19, 20]. In [10], the regularized term is the linear entropy among the joint measures. This work adds the term in the linear program while we put it into the optimal control. Moreover, the computation of the Benamou-Brenier formula has been discussed in [24] based on proximal splitting methods [3]. The proximal methods may take thousands of iterations while our Newton's method uses only about fifty steps.

The rest of paper is organized as follows: In section 2, we briefly review related problems in continuous space. We propose and analyze the discrete problem using Newton's method in section 3. Numerical examples are provided in section 4.

2. REVIEW

In this section, we briefly review optimal transport distance and its regularized problem.

Optimal transport distance provides a particular metric between two histograms. The problem was originally proposed by Monge in 1781 and then relaxed by Kantorovich in 1940s as follows: Given two densities ρ^0, ρ^1 supported on a compact, convex set $\Omega \subset \mathbb{R}^d$ with equal total mass, and $c : \Omega \times \Omega \rightarrow \mathbb{R}_+$ a ground cost function. Consider

$$\min_{\pi} \int_{\Omega \times \Omega} c(x, y) \pi(x, y) dx dy, \quad (1)$$

where the infimum is taken among all joint measures (transport plans) $\pi(x, y)$ having $\rho^0(x)$ and $\rho^1(y)$ as marginals, i.e.

$$\int_{\Omega} \pi(x, y) dy = \rho^0(x), \quad \int_{\Omega} \pi(x, y) dx = \rho^1(y), \quad \pi(x, y) \geq 0.$$

In numerics, (1) is a well known linear program, and many available techniques can be used. But they all involve a quadratic number of variables. E.g. if Ω is discretized into N points, the problem needs to solve a linear program with N^2 variables. This is difficult for applications whenever Ω belongs to a large dimensional space.

An equivalent formulation of (1) was initially introduced by Brenier and Benamou in 2000 [1]. It connects the original problem with an optimal control setting. Associate the

ground cost c with

$$c(x, y) := \inf_{\gamma} \left\{ \int_0^1 L(\dot{\gamma}(t)) dt : \gamma(0) = x, \gamma(1) = y \right\}, \quad (2)$$

where the infimum is taken among all possible continuous differentiable paths $\gamma(t)$ in Ω and L is assumed to be a strictly convex Lagrangian function. Then the optimal transport problem (1) can be formulated as

$$\inf_{m, \rho} \int_0^1 \int_{\Omega} L\left(\frac{m(t, x)}{\rho(t, x)}\right) \rho(t, x) dx dt, \quad (3)$$

where the infimum is taken among all Borel flux functions $m(t, x)$ with zero flux condition and density function $\rho(t, x)$, such that ρ^0 is continuously transported to ρ^1 by the continuity equation:

$$\frac{\partial \rho(t, x)}{\partial t} + \nabla \cdot m(t, x) = 0, \quad \rho(0, x) = \rho^0, \quad \rho(1, x) = \rho^1.$$

(3) is significant for computations. This is because (3) requires many fewer variables than (1), e.g. comparing $[0, 1] \times \Omega$ with $\Omega \times \Omega$. However, there are several difficulties associated with (3). One difficulty is that $\rho(t, x)$ may be 0, in which case the function $\frac{m(t, x)}{\rho(t, x)}$ is no longer smooth. This brings numerical difficulties and traditional optimization methods are not suitable.

In this paper, we focus on $c(x, y) = \|x - y\|^2$, $\|\cdot\|$ is a 2-norm, i.e. $L(\dot{\gamma}) = \|\dot{\gamma}\|^2$. In this case, the optimal transport distance is called the L^2 -Wasserstein metric. This choice of c leads to a connection with the following regularized problem: Parallel to Monge and Kantorovich, Schrödinger in 1931 discovered a similar transport problem, which is now called the *Schrödinger bridge problem* (SBP).

To illustrate, we focus on SBP in an optimal control setting: Given two strictly positive densities ρ^0, ρ^1 with equal mass, consider

$$\inf_{m, \rho} \int_0^1 \int_{\Omega} \frac{m^2(t, x)}{\rho(t, x)} dx dt, \quad (4)$$

where the infimum is taken among all drift flux function $m(t, x)$ with zero flux boundary condition and density function $\rho(t, x)$ with Neumann boundary condition, such that the Fokker-Planck equation holds

$$\frac{\partial \rho}{\partial t} + \nabla \cdot m(t, x) = \beta \Delta \rho, \quad \rho(0, x) = \rho^0, \quad \rho(1, x) = \rho^1.$$

The only difference between the optimal transport problem (3) and SBP (4) is the diffusion term in the controlled dynamical system. Recently many rigorous connections have been discovered. It was shown that the optimal value and minimizer of SBP converge to those of the L^2 -Wasserstein metric as $\beta \rightarrow 0$ in certain sense, see a review in [17]. Thus one may consider (4) as a regularized approximation of (3).

More importantly, there is an equivalent and crucial formulation of (4) discovered in [5, 29], which is essential for the computations throughout this paper. Consider

$$\inf_{m, \rho} \int_0^1 \int_{\Omega} \left\{ \frac{m^2(t, x)}{\rho(t, x)} + \beta^2 (\nabla \log \rho(t, x))^2 \rho(t, x) \right\} dx dt + 2\beta \mathcal{D}(\rho^1 | \rho^0), \quad (5)$$

where the infimum is taken among all flux function $m(t, x)$ and density function $\rho(t, x)$, such that the continuity equation holds

$$\frac{\partial \rho}{\partial t} + \nabla \cdot m(t, x) = 0, \quad \rho(0, x) = \rho^0, \quad \rho(1, x) = \rho^1.$$

Here m, ρ satisfies the same boundary conditions as in (4) and $\mathcal{D}(\rho^1 | \rho^0) := \int_{\Omega} \rho^1(x) \log \rho^1(x) dx - \int_{\Omega} \rho^0(x) \log \rho^0(x) dx$. Since the boundary densities ρ^0, ρ^1 are fixed, we treat \mathcal{D} as a constant in (5).

Derivation of (5). The main idea relating between (4) and (5) involves a change of variable. Construct a new flux function $\mathbf{m}(t, x)$ to represent the one $m(t, x)$ in (4):

$$\mathbf{m}(t, x) = m(t, x) - \beta \nabla \rho(t, x). \quad (6)$$

Substituting $\mathbf{m}(t, x)$ into (4), the problem is as follows. First, the Fokker-Planck equation is rewritten in terms of \mathbf{m} by a continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot m - \beta \Delta \rho = \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{m} = 0.$$

Second, following the observation

$$\nabla \rho = \rho \nabla \log \rho,$$

the SBP's cost functional becomes

$$\begin{aligned} \int_0^1 \int_{\Omega} \frac{m^2}{\rho} dx dt &= \int_0^1 \int_{\Omega} \frac{(\mathbf{m} + \beta \nabla \rho)^2}{\rho} dx dt = \int_0^1 \int_{\Omega} \frac{(\mathbf{m} + \beta \rho \nabla \log \rho)^2}{\rho} dx dt \\ &= \int_0^1 \int_{\Omega} \left\{ \frac{\mathbf{m}^2}{\rho} + \beta^2 (\nabla \log \rho)^2 \rho + 2\beta \mathbf{m} \cdot \nabla \log \rho \right\} dx dt. \end{aligned}$$

We claim that the coefficient of β is a constant. Since

$$\begin{aligned} &\int_0^1 \int_{\Omega} \mathbf{m} \cdot \nabla \log \rho dx dt \\ &= - \int_0^1 \int_{\Omega} \log \rho \nabla \cdot \mathbf{m} dx dt && \text{Integration by parts w.r.t. } x \\ &= \int_0^1 \int_{\Omega} \log \rho \frac{\partial \rho}{\partial t} dx dt = \int_{\Omega} \int_0^1 \log \rho \frac{\partial \rho}{\partial t} dt dx && \text{Fubini's theorem} \\ &= \int_{\Omega} \rho \log \rho \Big|_{t=0}^{t=1} dx - \int_0^1 \int_{\Omega} \rho \frac{\partial}{\partial t} \log \rho dx dt && \text{Integration by parts w.r.t } t \\ &= \int_{\Omega} \{ \rho^1 \log \rho^1 - \rho^0 \log \rho^0 \} dx - \int_0^1 \int_{\Omega} \frac{1}{\rho} \cdot \rho \cdot \frac{\partial \rho}{\partial t} dx dt \\ &= \int_{\Omega} \{ \rho^1(x) \log \rho^1(x) - \rho^0(x) \log \rho^0(x) \} dx \\ &= \text{Constant} \end{aligned}$$

where the second last equality comes from the spatial integration by parts: notice that m has a zero flux condition, then $\int_{\Omega} \frac{\partial \rho}{\partial t} dx = - \int_{\Omega} \nabla \cdot m dx = 0$. Combining the above three steps and denoting \mathbf{m} by m , we finish the derivation. \square

(5) is the main problem considered in this paper. In this formulation, the main difference between (3) and (5) is

$$\mathcal{I}(\rho) = \int_{\mathbb{R}^d} (\nabla \log \rho(x))^2 \rho(x) dx ,$$

which is named *Fisher information*. In physics and engineering studies, \mathcal{I} is a fundamental functional [13]. Nice properties involving Fisher information, diffusion processes and optimal transport theory have been discussed [30]. Here we apply Fisher information as the regularized term, and focus on its following numerical advantages:

- (i) \mathcal{I} keeps the density function strictly positive in the minimization;
- (ii) \mathcal{I} brings strict convexity to the original optimal transport problem.

In next section, we shall design a fast and simple algorithm to solve (5), and adopt its solution to approximate the one in L^2 -Wasserstein metric. This idea can be generalized for any ground cost c , see details in the discussion section.

3. ALGORITHM

In this section, we form (5) as a finite dimensional minimization problem using the discretization developed in [7, 8, 14, 18]. The discretized problem is shown to be smooth and strictly convex, so that Newton's method can be applied.

3.1. Problem formulation. We start with applying a finite graph to discretize the spatial domain $\Omega \subset \mathbb{R}^d$. For concreteness, assume that $\Omega = [0, 1]^d$ and $G = (V, E)$ is a uniform lattice graph with equal spacing $\Delta x = \frac{1}{n}$ on each dimension. Here V is a vertex set with $N = (n+1)^d$ nodes, and each node, $i = (i_k)_{k=1}^d \in V$, $1 \leq k \leq d$, $0 \leq i_k \leq n$, represents a cube with length Δx :

$$C_i(x) = \{(x_1, \dots, x_d) \in [0, 1]^d : |x_1 - i_1 \Delta x| \leq \Delta x/2, \dots, |x_d - i_d \Delta x| \leq \Delta x/2\} ;$$

E is an edge set, where $i + \frac{e_v}{2} := \text{edge}(i, i + e_v)$ and e_v is a unit vector at v -th column.

Denote a discrete probability set

$$\mathcal{P}(G) = \{p = (p_i)_{i \in V} : \sum_{i \in V} p_i = 1, p_i \geq 0, i \in V\} ,$$

where p_i represents a probability on node i , i.e.

$$p_i \approx \int_{C_i(x)} \rho(x) dx ,$$

where $\rho(x)$ is the density function in continuous space. The interior of $\mathcal{P}(G)$, the set of all strictly positive measures, is denoted by $\mathcal{P}_o(G)$. Assume two given measures $p^0 = (p_i^0)_{i \in V}$, $p^1 = (p_i^1)_{i \in V} \in \mathcal{P}_o(G)$.

Let the discrete flux function be $m = (m_{i+\frac{e_v}{2}})_{i+\frac{e_v}{2} \in E}$, where $m_{i+\frac{e_v}{2}}$ represents the discrete flux on the edge $i + \frac{e_v}{2}$, i.e.

$$m_{i+\frac{e_v}{2}} \approx \int_{C_{i+\frac{e_v}{2}}(x)} m_v(x) dx ,$$

where $m(x) = (m_1(x), \dots, m_v(x), \dots, m_d(x))$ is the flux function in continuous space. The discrete zero flux condition is described as follows:

$$m_{i+\frac{e_v}{2}} = 0, \quad \text{if } i = (i_k)_{k=1}^d \text{ with } i_k = 0 \text{ or } n, \text{ for } k = 1, \dots, d.$$

We propose the cost functional and constraint for (5) by using the following definitions. The discrete divergence operator is:

$$\operatorname{div}(m)|_i = \frac{1}{\Delta x} \sum_{v=1}^d (m_{i+\frac{1}{2}e_v} - m_{i-\frac{1}{2}e_v}).$$

The discretized cost functional needs special treatment [7, 8]. Take the kinetic energy

$$\mathcal{K}(m, p) = \sum_{i+\frac{e_v}{2} \in E} \frac{m_{i+\frac{1}{2}e_v}^2}{g_{i+\frac{1}{2}e_v}},$$

and the discrete Fisher information

$$\mathcal{I}(p) := \sum_{i+\frac{e_v}{2} \in E} \frac{1}{\Delta x^2} (\log p_i - \log p_{i+e_v})^2 g_{i+\frac{1}{2}e_v},$$

where $g_{i+\frac{1}{2}e_v} := \frac{1}{2}(p_i + p_{i+e_v})$ is the discrete probability on edge $i + \frac{e_v}{2} \in E$, which is a simple average of discrete measures supported at nodes i and $i + e_v$. The choice of $g_{i+\frac{1}{2}e_v}$ is not unique. For example, it can be a logarithmic mean of p_i, p_{i+e_v} . But representing probabilities as a weight on the edge is necessary, since it allows the discrete integration by parts formula with respect to a discrete measure, see [7] for details.

We further introduce a time discretization. The time interval $[0, 1]$ is divided into L intervals with endpoints $t_l = l * \Delta t$, $\Delta t = \frac{1}{L+1}$, $l = 0, 1, \dots, L, L+1$. Thus $\rho(t, x)$, $m(t, x)$ are represented by $p = (p_{i,l}) \in \mathbb{R}^{|V|L}$, $m = (m_{i+\frac{e_v}{2},l}) \in \mathbb{R}^{|E|L}$, where $1 \leq i \leq N$, $1 \leq l \leq L$ and $|V|, |E|$ are numbers of vertices, edges respectively.

Combining the above spatial discretization and a forward finite difference scheme on time variable, we arrive at the **discretized Schrödinger bridge problem**:

$$\min_{m,p} \sum_{l=1}^L \sum_{i+\frac{e_v}{2} \in E} \left\{ \frac{m_{i+\frac{e_v}{2},l}^2}{(p_{i,l} + p_{i+e_v,l})/2} + \frac{\beta^2}{\Delta x^2} (\log p_{i,l} - \log p_{i+e_v,l})^2 \frac{p_{i,l} + p_{i+e_v,l}}{2} \right\}$$

subject to

$$p_{i,l} \geq 0;$$

$$\frac{p_{i,l+1} - p_{i,l}}{\Delta t} + \frac{1}{\Delta x} \sum_{v=1}^d (m_{i+\frac{1}{2}e_v,l} - m_{i-\frac{1}{2}e_v,l}) = 0;$$

$$p_{i,0} = p_i^0, \quad p_{i,L+1} = p_i^1, \quad i \in V, \quad l = 1, \dots, L.$$

(7)

3.2. Properties of the discretized problem. (7) is a finite dimensional optimization problem, which contains both equality and inequality constraints. We demonstrate that the discrete Fisher information plays the role of penalty function, which is similar to the one used in barrier methods for constrained optimization.

For simplicity, we denote (7) by

$$\min \left\{ \sum_{l=1}^T \mathcal{K}(m, p)|_l + \beta^2 \mathcal{I}(p)|_l : (m, p) \in \Theta \right\},$$

where the notation $|_l$ represents the cost functional at time t_l , and the constraint set forms

$$\Theta = \{(m, p) \in \mathbb{R}^{|E|L} \times \mathbb{R}^{|V|L} : (m, p) \text{ satisfies (7)}\}.$$

The interior of the feasible set Θ is

$$\text{interior}(\Theta) = \{(m, p) : (m, p) \in \Theta \text{ and } p_{i,l} > 0, \text{ for any } i \in V, l = 1, \dots, L\}.$$

In the following theorem, we show that (7) has certain good properties, which allows us to apply Newton's method [16].

Theorem 1. *The objective function of problem (7) is strictly convex for $(m, p) \in \text{interior}(\Theta)$. Moreover, the minimizer $(m^*, p^*) \in \text{interior}(\Theta)$ is unique.*

The main idea of the proof is as follows. Since the objective function is a summation of functions on each time t_l , we only need to estimate $\mathcal{K}(m, p) + \beta^2 \mathcal{I}(p)$, where p represents a vector in $\mathbb{R}^{|V|}$ for fixed level l .

- (1) We show that I becomes positive infinity on the boundary of the probability set. This lets us to conclude that the minimizer is obtained in the $\text{interior}(\Theta)$.

Lemma 2. $\mathcal{I}(p) = +\infty$, if $p \in \mathcal{P}(G) \setminus \mathcal{P}_o(G)$.

- (2) We prove strict convexity of the objective function in the $\text{interior}(\Theta)$.

Lemma 3. $\mathcal{K}(m, p) + \beta^2 \mathcal{I}(p)$ is strictly convex in the $\text{interior}(\Theta)$.

We let $N(i)$ represent the adjacent set in G , neighborhood of node i , i.e. $N(i) = \{j \in V : \text{edge}(i, j) \in E\}$.

Proof of Lemma 2. We show that $\mathcal{I}(p)$ is positive infinity on the boundary, i.e.

$$\lim_{\min_{i \in V} p_i \rightarrow 0} \mathcal{I}(p) = +\infty.$$

Suppose the above is not true, there exists a constant $M > 0$, such that if there exists some $i^* \in V$, $p_{i^*} = 0$, then

$$\begin{aligned} M \geq \mathcal{I}(p) &= \sum_{i+\frac{e_v}{2} \in E} \frac{1}{\Delta x^2} (\log p_i - \log p_{i+e_v})^2 \frac{p_i + p_{i+e_v}}{2} \\ &\geq \sum_{i+\frac{e_v}{2} \in E} \frac{1}{\Delta x^2} (\log p_i - \log p_{i+e_v})^2 \frac{1}{2} \max\{p_i, p_{i+e_v}\}. \end{aligned} \quad (8)$$

Each term in (8) is non-negative, thus

$$(\log p_i - \log p_{i+e_v})^2 \max\{p_i, p_{i+e_v}\} \leq 2M < +\infty,$$

for any $\text{edge}(i, i+e_v) \in E$. Since $p_{i^*} = 0$, the above formula further implies that for any $\tilde{i} \in N(i^*)$, $p_{\tilde{i}} = 0$. This is true since if $p_{i^*} \neq 0$, we have

$$\lim_{p_{i^*} \rightarrow 0} (\log p_{i^*} - \log p_{\tilde{i}})^2 \max\{p_{i^*}, p_{\tilde{i}}\} = +\infty.$$

Similarly, we show that for any nodes $\tilde{\tilde{i}} \in N(\tilde{i})$, $p_{\tilde{\tilde{i}}} = 0$. We iterate the above steps a finite number of times. Since the lattice graph is connected and the set V is finite, we obtain $p_i = 0$, for any $i \in V$. This contradicts the assumption that $\sum_{i \in V} p_i = 1$, which finishes the proof. \square

Proof of Lemma 3. We prove that $\mathcal{K}(m, p) + \beta^2 \mathcal{I}(p)$ is strictly convex in the interior(Θ) by the following two steps.

First, we show that $\mathcal{I}(p)$ is strictly convex in the variable p with a constraint $\sum_{i \in V} p_i = 1$, $p_i > 0$, for any $i \in V$. We shall show

$$\min_{\sigma} \{ \sigma^T \mathcal{I}_{pp} \sigma : \sigma^T \sigma = 1, \sum_{i \in V} \sigma_i = 0 \} > 0. \quad (9)$$

Here $\mathcal{I}_{pp} = (\frac{\partial^2}{\partial p_i \partial p_j} \mathcal{I}(p))_{i \in V, j \in V} \in \mathbb{R}^{|V| \times |V|}$, and $\sum_{i \in V} \sigma_i = 0$ is the constraint for p lying on the simplex set $\mathcal{P}_o(G)$.

By direct computations,

$$\frac{\partial^2}{\partial p_i \partial p_j} \mathcal{I}(p) = \begin{cases} -\frac{1}{p_i p_j} \frac{1}{\Delta x^2} t_{ij} & \text{if } j \in N(i); \\ \frac{1}{p_i^2} \sum_{k \in N(i)} \frac{1}{\Delta x^2} t_{ik} & \text{if } i = j; \\ 0 & \text{otherwise,} \end{cases} \quad (10)$$

where

$$t_{ij} = (p_i - p_j)(\log p_i - \log p_j) + (p_i + p_j) > 0.$$

Hence

$$\begin{aligned} \sigma^T \mathcal{I}_{pp}(p) \sigma &= \frac{1}{2} \sum_{(i,j) \in E} t_{ij} \left\{ \left(\frac{\sigma_i}{p_i} \right)^2 + \left(\frac{\sigma_j}{p_j} \right)^2 - 2 \frac{\sigma_i}{p_i} \frac{\sigma_j}{p_j} \right\} \\ &= \frac{1}{2} \sum_{(i,j) \in E} t_{ij} \left(\frac{\sigma_i}{p_i} - \frac{\sigma_j}{p_j} \right)^2 \geq 0, \end{aligned}$$

where $\frac{1}{2}$ is due to the convention that each edge $(i, j) \in E$ is summarized twice.

We next show that the strict inequality in (9) holds. Suppose (9) is not true, there exists a unit vector σ^* such that

$$\sigma^{*T} \mathcal{I}_{pp} \sigma^* = \frac{1}{2} \sum_{(i,j) \in E} t_{ij} \left(\frac{\sigma_i^*}{p_i} - \frac{\sigma_j^*}{p_j} \right)^2 = 0.$$

Then $\frac{\sigma_1^*}{p_1} = \frac{\sigma_2^*}{p_2} = \dots = \frac{\sigma_n^*}{p_{|V|}}$. Combining this with the constraint $\sum_{i \in V} \sigma_i^* = 0$, we have $\sigma_1^* = \sigma_2^* = \dots = \sigma_{|V|}^* = 0$, which contradicts that σ^* is a unit vector. \square

Secondly, we prove that $\mathcal{K}(m, p) + \beta^2 \mathcal{I}(p)$ is strictly convex in (m, p) . Since (m, p) is in the interior, we have $p_i > 0$, thus the objective function is smooth. We shall show that

$$\lambda(m, p) > 0, \quad \text{for any } (m, p) \in \text{interior}(\Theta),$$

where

$$\lambda(m, p) := \min_{h, \sigma} \begin{pmatrix} h \\ \sigma \end{pmatrix}^T \left\{ \begin{pmatrix} \mathcal{K}_{mm} & \mathcal{K}_{mp} \\ \mathcal{K}_{pm} & \mathcal{K}_{pp} \end{pmatrix} + \beta^2 \begin{pmatrix} 0 & 0 \\ 0 & \mathcal{I}_{pp} \end{pmatrix} \right\} \begin{pmatrix} h \\ \sigma \end{pmatrix} \quad (11)$$

subject to

$$h \in \mathbb{R}^{|E|}, \quad \sigma \in \mathbb{R}^{|V|}, \quad h^T h + \sigma^T \sigma = 1, \quad \sum_{i \in V} \sigma_i = 0.$$

Here $\lambda(m, p)$ is the smallest eigenvalue of Hessian matrix for the objective function on the interior of constraint Θ , with tangent vectors (h, σ) .

We show that $\mathcal{K}(m, p)$ is a smooth, convex function in interior of Θ . We have

$$\mathcal{K}(m, p) = \sum_{i + \frac{e_v}{2} \in E} \frac{2m_{i + \frac{e_v}{2}}^2}{p_i + p_{i+e_v}}.$$

Since $\frac{x^2}{y}$ is convex when $y > 0$ and $p_i + p_{i+e_v}$ is concave on variables $p_i, p_{i+e_v} > 0$. Then \mathcal{K} is convex. From (9), we have

$$\mathcal{J}(h, \sigma) := \begin{pmatrix} h \\ \sigma \end{pmatrix}^T \begin{pmatrix} \mathcal{K}_{mm} & \mathcal{K}_{mp} \\ \mathcal{K}_{pm} & \mathcal{K}_{pp} \end{pmatrix} \begin{pmatrix} h \\ \sigma \end{pmatrix} + \beta^2 \sigma^T \mathcal{I}_{pp} \sigma \geq 0. \quad (12)$$

We claim that the inequality in (12) is strict. Suppose there exists (h^*, σ^*) , such that (12) is zero, i.e.

$$\mathcal{J}(h^*, \sigma^*) = 0.$$

In this case, from (9), $\sigma^* = 0$. Thus (12) forms

$$\mathcal{J}(h^*, \sigma^*) = h^{*T} \mathcal{K}_{mm} h^* = 0.$$

Since $\mathcal{K}_{mm} = \text{diag}(\frac{4}{p_i + p_{i+e_v}})_{i + \frac{e_v}{2} \in E}$ is strictly positive, we have $h^* = 0$, which contradicts the fact that $h^T h + \sigma^T \sigma = 1$.

Proof of Theorem 1. It is now easy to prove Theorem 1. From Lemma 2, we know the minimizer of (7) is taken in the interior of the constraint set. Following Lemma 3, (7) has a unique minimizer. \square

3.3. Algorithm. We are ready to present the proximal Newton's method for (7) based on Theorem 1. The general setting of the proximal Newton's method is as following. Let us concatenate m and p together and introduce the new variable $u = (m, p)^T \in \mathbb{R}^{|E|L+|V|L}$. The problem (7) can be then formulated as

$$\min_u f(u) \quad \text{subject to} \quad Au = b, \quad p \geq 0,$$

where $f : \mathbb{R}^{|E|L+|V|L} \rightarrow \mathbb{R}_+$ is the objective function of (7), $A \in \mathbb{R}^{|E|L+|V|L}$, $b \in \mathbb{R}^{|V|L}$ are used for representing linear constraints of (7), and $p \geq 0$ enforces $p_{i,l} \geq 0$.

At the k -th iteration, the proximal Newton's method first minimizes the quadratic approximation of f around u^k by ignoring a constant:

$$\min_u (u - u^k)^T \nabla f(u^k) + \frac{1}{2} (u - u^k)^T H_k (u - u^k) \quad \text{subject to} \quad Au = b,$$

where $H_k \in \mathbb{R}^{|E|L+|V|L \times |E|L+|V|L}$ is the Hessian matrix of f at u^k . Because $Au^k = b$, the above constrained optimization is equivalent to solving

$$d^k = \arg \min_d d^T \nabla f(u^k) + \frac{1}{2} d^T H_k d \quad \text{subject to} \quad Ad = 0. \quad (13)$$

Then d^k serves as the search direction, and u^{k+1} is updated as

$$u^{k+1} = u^k + \alpha_k d^k$$

with some step size $\alpha_k > 0$.

In addition, there are several important computational remarks. First, a feasible solution $u^0 = (m^0, p^0) \in \Theta$ is needed. This can be done using the following approach:

- (1) Consider p^0 as the time linear interpolation of p^0, p^1 :

$$p_{i,l}^0 = (1 - t_l)p_i^0 + t_l p_i^1 ; \quad (14)$$

- (2) Construct the discrete flux function m by a discrete gradient function. Denote a vector $\Phi \in \mathbb{R}^{|V|L}$. We form

$$m_{i+\frac{e_v}{2},l}^0 = \Phi_{i+e_v,l} - \Phi_{i,l} , \quad (15)$$

where Φ satisfies

$$\frac{p_{i,l+1}^0 - p_{i,l}^0}{\Delta t} + \sum_{v=1}^d \sum_{i+\frac{e_v}{2} \in E} (\Phi_{i+e_v,l} - \Phi_{i,l}) = 0 .$$

By solving the above linear equations, m^0 is uniquely determined.

Under this approach, $p_{i,l}^0 > 0$ since (14) holds when p_i^0, p_i^1 are positive. Thus $(m^0, p^0) \in \text{interior}(\Theta)$.

Second, A is the discrete divergence operator, w.r.t. (t, x) . The projection operator to (7)'s linear constraint, used in initialization and Newton step (13), can be dealt with by solving a discrete elliptic equation, where the fast Fourier transform method is available [24].

Last, the Hessian matrix H_k is a highly sparse matrix. This is because the objective function f is a summation of each spatial (edge) and time level. Thus the nonzero entries of Hessian matrix exist only on each edge and time level t_l . This is especially true for the Hessian operator of Fisher information reported in (10).

Based the above discussion, the proposed algorithm is as follows:

Proximal Newton Method for Wasserstein metric

Input: Discrete probabilities p^0, p^1 ;

Parameter $\beta > 0$, step size $\alpha_k \in (0, 1)$, discretization parameters $\Delta x, \Delta t$, $\theta \in [0, 1]$.

Output: The minimizer $u^* = (m^*, p^*)$ and minimal value $f(u^*)$.

0. Follow (14), (15) find a feasible path $u^0 = (m^0, p^0)^T$;
 1. **for** $k = 1, 2, \dots$ while not converged
 2. $d^k = \arg \min_d d^T \nabla f(u^k) + \frac{1}{2} d^T H_k d$ subject to $Ad = 0$;
 3. $u^{k+1} = u^k + \alpha_k d^k$.
 4. **end**
-

Based on Theorem 1, the minimizer of (7) is taken in the interior of Θ , in which f is smooth and strongly convex (in the neighborhood of minimizer). The computational cost per iteration lies in the quadratic programming subproblem in line 3, where we can take advantage of the sparsity of H_k . The proximal Newton method has q -quadratic convergence rate when the objective function is strongly convex and step size is chosen sufficiently small. We refer readers to [16] for details.

Remark 1. Here the strict positivity condition on p^0, p^1 can be relaxed. The optimization problem (7) is still valid even if p^0, p^1 are not strictly positive. In this case, Theorem 1 ensures that the computed path $p_{i,l}$ is strictly positive, for $1 \leq l \leq L$.

Remark 2. It is also worth noting that the Fisher information introduces an important convexity into minimization (7), see details in (12). This is because that the Hessian matrix of Fisher information, shown in (10), introduces a graph Laplacian like matrix, whose smallest positive eigenvalue ensures the quadratic convergence rate of the proposed Newton's method.

4. NUMERICAL EXAMPLES

In this section, we present several numerical examples using MATLAB to demonstrate the effectiveness of the proposed method. Throughout the experiments, we adopted a step size $\alpha_k \equiv 0.3$, and the following stopping criterion for the algorithm

$$\frac{|f(u^{k+1}) - f(u^k)|}{|f(u^k)|} < 10^{-5}.$$

We used regularization parameter $\beta^2 = 10^{-6}$ for all experiments except $\beta^2 = 10^{-5}$ in Example 3. We show curves of objective values versus iteration number for all examples, and plot the status of the density at different time.

We first show a one-dimensional synthetic example. Specifically, we consider the densities

$$p_i^0 = \exp\left(-\frac{(x_i - 0.4)^2}{0.01}\right) + 0.01, \quad p_i^1 = \exp\left(-\frac{(x_i - 1.6)^2}{0.01}\right) + 0.01,$$

on the interval $[0, 2]$. The space and time were discretized uniformly with $N = 40$ and $T = 50$ with $x_i = \frac{i}{20}$. We normalized p^0 and p^1 so that $\sum_{i \in V} p_i^0 = \sum_{i \in V} p_i^1 = 1$.

The second example is similar to example 1, but in a two-dimensional case. Let

$$p_i^0 = \exp\left(-\frac{\|x_i - (0.2, 0.5)\|^2}{0.01}\right) + 0.01, \quad p_i^1 = \exp\left(-\frac{\|x_i - (1.5, 1.5)\|^2}{0.01}\right) + 0.01$$

be defined on $[0, 2] \times [0, 2]$. We adopted spatial and time discretization with $N = 20^2$ and $T = 30$, $x_i = (\frac{i_1}{10}, \frac{i_2}{10})$, and normalized the densities so that $\sum_{i \in V} p_i^0 = \sum_{i \in V} p_i^1 = 1$.

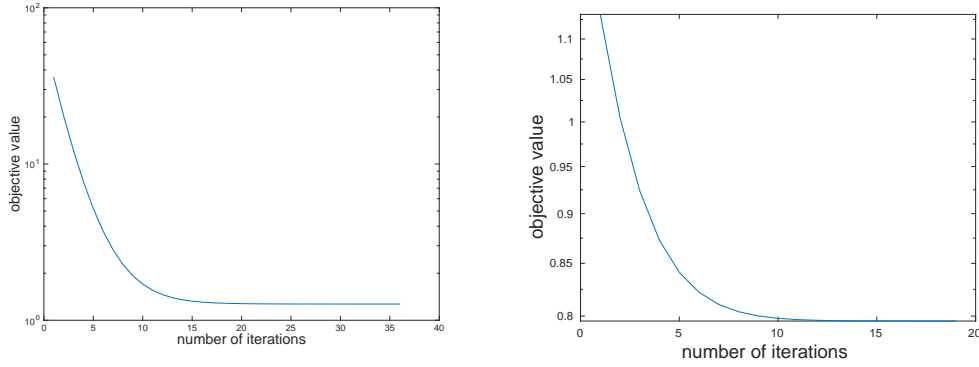


FIGURE 1. Curves of objective value versus iteration numbers for Example 1 (left) and Example 2 (right).

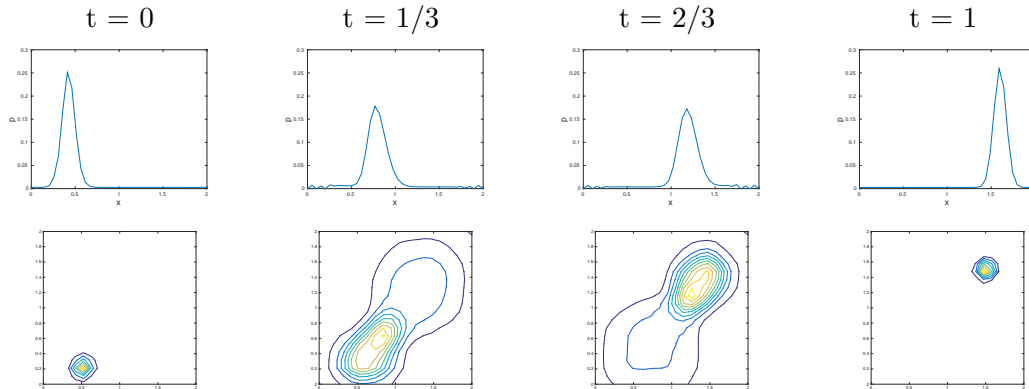


FIGURE 2. The density p at different time. Left: contour plots of p in Example 1. Right: contour plots of p in Example 2.

In what follows, we present two gray-scale image examples. In Example 3, a square is smoothly split into two; see Fig. 4. In the last example, we used two images from the MNIST database of handwritten digits [15]. One is a image of handwritten ‘4’ and the other is ‘1’. The images are of size 28×28 , and the time space is discretized using $L = 30$. The results are shown in Fig. 3 and 5. It can be seen that the initial image is continuously transported to the other. As we have observed, adding Fisher information (diffusion process) reduces the number of computation iterations drastically. However it also blurs each frame of the movie. One can use further image denoising techniques to remove the noise in each frame, e.g. [26].

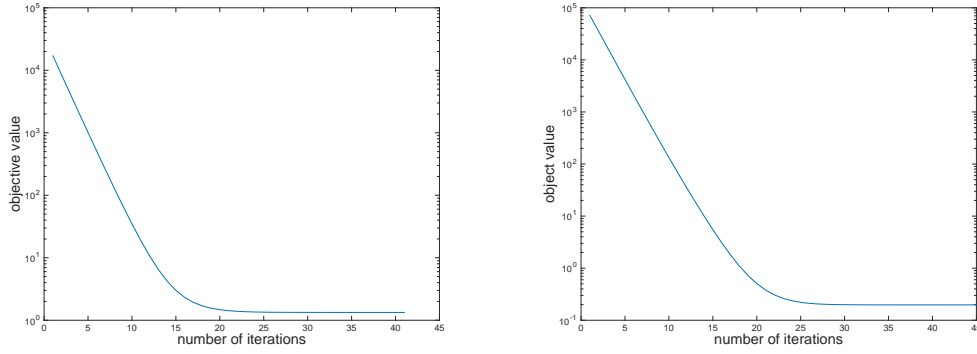


FIGURE 3. Curves of objective value versus iteration numbers for Example 3 (left) and Example 4 (right).

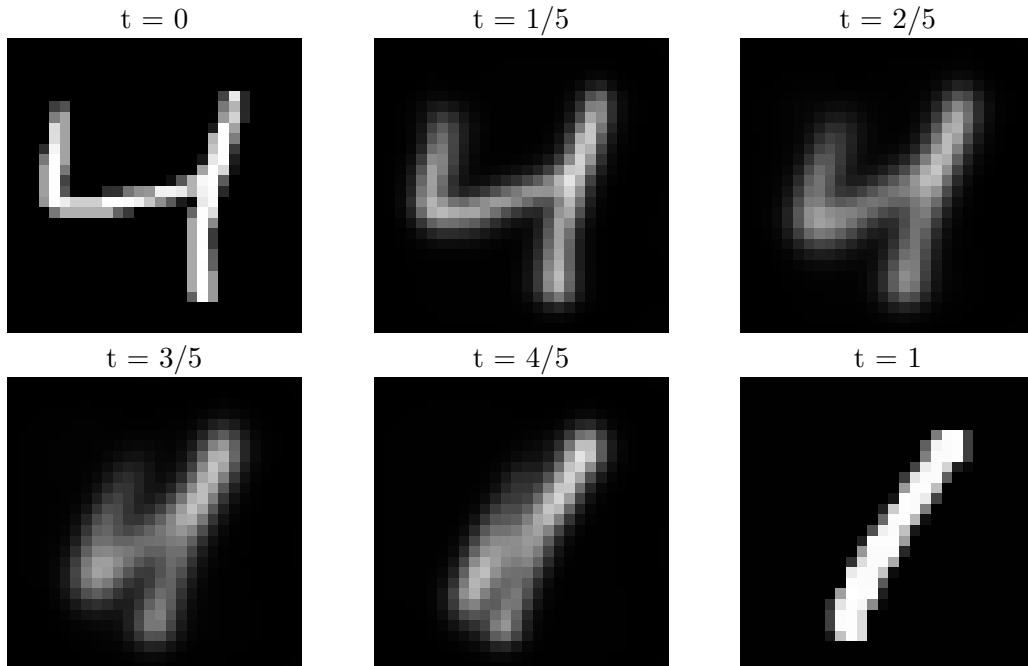


FIGURE 4. Motions for Example 3

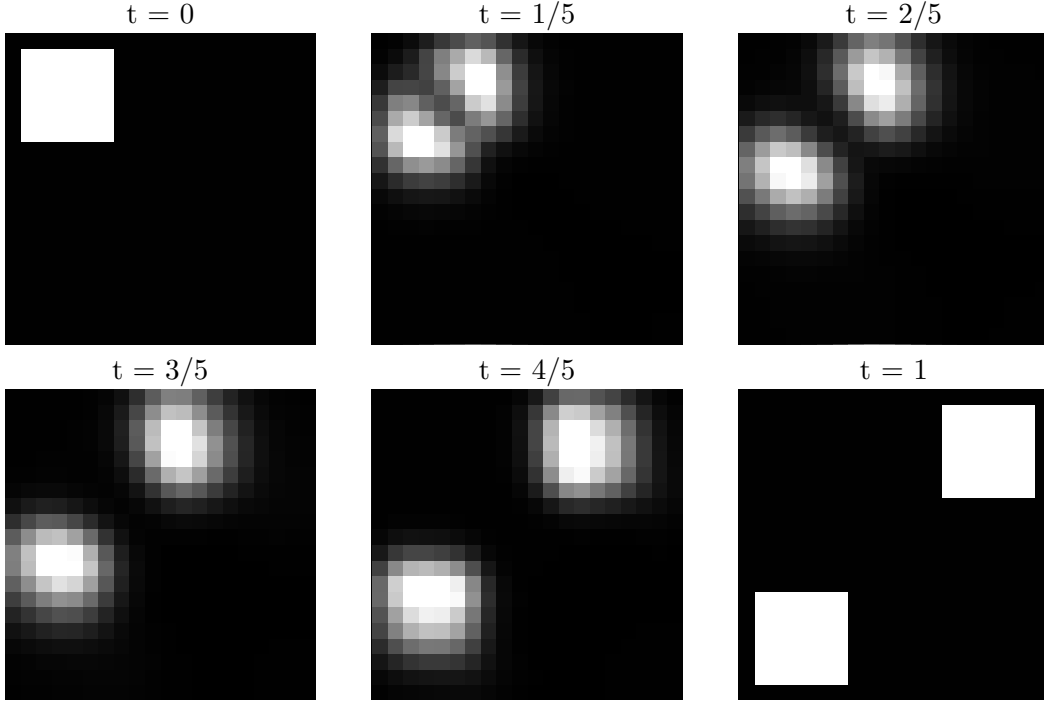


FIGURE 5. Motions for MNIST example

5. DISCUSSION

In this paper, we proposed a new model for L^2 -Wasserstein metric using regularization via Fisher information. The regularized term brings strict convexity to the original problem and handles its inequality constraints.

In fact, the Fisher information can be used for computations of optimal transport distance with a generalized ground cost. E.g. associating c with a Lagrange function L in (2), we introduce a regularized minimization:

$$\inf_{m, \rho} \left\{ \int_0^1 \int_{\Omega} \left[L\left(\frac{m}{\rho}\right) dx + \beta^2 \mathcal{I}(\rho) \right] dx dt : \frac{\partial \rho}{\partial t} + \nabla \cdot m = 0, \rho(0, x) = \rho^0, \rho(1, x) = \rho^1 \right\},$$

where β is a small positive constant and \mathcal{I} is the Fisher information. In this case, a discretized problem similar to (7) can be introduced, and Theorem 1 holds under suitable conditions of L .

In future work, we shall continue to study some theoretical questions introduced by the model. E.g. (1) How does the discretized minimization approximate the continuous limit? (2) For general ground cost, what is the effect of Fisher information on the original problem's minimizer and minimal value when β goes to zero.

Acknowledgement: We would like to thank Professors Shui-Nee Chow, Wilfrid Gangbo and Haomin Zhou for many discussions on related topics.

REFERENCES

- [1] Jean-David Benamou and Yann Brenier. A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem. *Numerische Mathematik* 84(3): 375–393, 2000.
- [2] Eric Carlen. Stochastic mechanics: a look back and a look ahead. *Diffusion, quantum theory and radically elementary mathematics*, 47: 117–139, 2014.
- [3] Antonin Chambolle, and Thomas Pock. A first-order primal-dual algorithm for convex problems with applications to imaging. *Journal of Mathematical Imaging and Vision* 40(1):120–145, 2011.
- [4] Lenaïc Chizat, Gabriel Peyré, Bernhard Schmitzer and François-Xavier Vialard. An Interpolating Distance Between Optimal Transport and Fisher–Rao Metrics, *Foundations of Computational Mathematics*, 1–44, Springer, 2016.
- [5] Yongxin Chen, Tryphon Georgiou and Michele Pavon. On the relation between optimal transport and Schrödinger bridges: A stochastic control viewpoint. *Journal of Optimization Theory and Applications*, 169(2): 671–691, 2016.
- [6] Shui-Nee Chow, Wen Huang, Yao Li, and Haomin Zhou. Fokker–Planck equations for a free energy functional or Markov process on a graph. *Archive for Rational Mechanics and Analysis*, 203(3):969–1008, 2012.
- [7] Shui-Nee Chow, Wuchen Li and Haomin Zhou. Nonlinear Fokker-Planck Equations on Finite Graphs and their asymptotic properties, *arXiv:1701.04841*, 2016.
- [8] Shui-Nee Chow, Luca Dieci, Wuchen Li and Haomin Zhou. Entropy dissipation semi-discretization schemes for Fokker-Planck equations, *arXiv:1608.02628*, 2016.
- [9] Shui-Nee Chow, Wuchen Li and Haomin Zhou. Schrödinger equation on a graph via optimal transport, 2017.
- [10] M. Cuturi. Sinkhorn distances: Lightspeed computation of optimal transport. In *Conference on Neural Information Processing Systems (NIPS13)*, 2292–2300, 2013.
- [11] Lawrence Evans. Partial differential equations and Monge-Kantorovich mass transfer. *Current developments in mathematics* (1) 65–126, 1997.
- [12] Lawrence Evans and Wilfrid Gangbo. Differential equations methods for the Monge-Kantorovich mass transfer problem. *Memoirs of AMS*, no 653, vol. 137, 1999.
- [13] B. Roy Frieden. *Science from Fisher Information: A Unification*, Cambridge University Press, 2004.
- [14] Wilfrid Gangbo, Wuchen Li and Chenchen Mou. Schrödinger bridge problem on a graph via optimal transport, 2017.
- [15] Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. *Gradient-based learning applied to document recognition*, *Proceedings of the IEEE*, 86(11):2278–2324, 1998.
- [16] Jason D. Lee, Yuekai Sun, and Michael A. Saunders. Proximal Newton-type methods for convex optimization. *NIPS*. Vol. 25. 2012.
- [17] Christian Léonard. A survey of the Schrödinger problem and some of its connections with optimal transport. *arXiv preprint arXiv:1308.0215*, 2013.
- [18] Wuchen Li. A study of stochastic differential equations and Fokker-Planck equations with applications. *PhD thesis*, 2016.
- [19] Wuchen Li, Ernest Ryu, Stanley Osher, Wotao Yin, and Wilfrid Gangbo. A Fast algorithm for Earth Mover’s Distance based on optimal transport and L_1 type Regularization. *arXiv:1609.07092*, 2016.
- [20] Wuchen Li, Penghang Yin and Stanley Osher. A Fast algorithm for unbalanced L_1 Monge-Kantorovich problem. *CAM report*, 2016.
- [21] Jan Maas. Gradient flows of the entropy for finite Markov chains. *Journal of Functional Analysis*, 261(8):2250–2292, 2011.
- [22] L. Métivier, R. Brossier, Q. Mérigot, E. Oudet and J. Virieux. Measuring the misfit between seismograms using an optimal transport distance: application to full waveform inversion. *Geophysical Journal International*, (205) 1: 345–377, 2016.
- [23] Edward Nelson. Derivation of the Schrödinger Equation from Newtonian Mechanics, *Physical Review* 150 (4): 1079, 1966.
- [24] Nicolas Papadakis, Gabriel Peyré and Edouard Oudet, Optimal transport with proximal splitting, *SIAM Journal on Imaging Sciences* 7(1): 212–238, SIAM, 2014.
- [25] Yossi Rubner, Carlo Tomasi and Leonidas Guibas. The Earth mover’s distance as a metric for image retrieval. *International journal of computer vision*, 40(2): 99–121, 2000.
- [26] Leonid Rudin, Stanley Osher and Emad Fatemi. Nonlinear total variation based noise removal algorithms, *Physica D: Nonlinear Phenomena*, (60) 259–268, 1992.

- [27] Filippo Santambrogio. Optimal transport for applied mathematicians. *Birkuser*, 2015.
- [28] E. Schrödinger. Quantisierung als Eigenwertproblem (zweite Mitteilung). *Annalen der Physik* 79, 489–527, 1926.
- [29] Kunio Yasue. Stochastic calculus of variations. *Journal of functional Analysis*, 327-340, 1981.
- [30] Cédric Villani. *Optimal transport: old and new*, volume 338. Springer Science & Business Media, 2008.